Affinity of disperse dyes on polyester fibers in non-aqueous media: effect of substituents in terms of the electric dipole moments

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Various attempts for non-aqueous dyeing systems, especially towards polyester substrates, have been carried out to investigate fundamental exhaustion properties of disperse dyes. A wide range of non-aqueous solvents as possible exhaustion media were surveyed to examine the adsorption and the solubility properties.

In this work, the effects of the chemical structures of the disperse dyes on adsorption affinity were investigated with relation to hydrophobic or hydrophilic characteristics of dye substituents. Azo and anthraquinone dyes having different substituents were examined using 5 kinds of representative non-aqueous adsorption media and the adsorption affinity in pentane was then discussed with relation to both chemical structure and solubility of the dyes. In addition, the solubility of the disperse dyes in pentane was surveyed with respect to dipole moments of the dyes caused by their dye structural substituents. Generally, the dipole moment of dyes measures the asymmetrical states in the molecular charge distribution. Also this value represents a sum of vectors from three dimensional calculations. Therefore, it can be considered as the polarity of each molecule. It is proposed that the dipole moment of the dyes resulting from the different chemical structures exhibits the changes of hydrophilicity or hydrophobicity. Consequently, the dipole moment properties provide the solubility changes of the dyes in hydrophobic pentane medium. However, it is very difficult to determine the exact dipole moments using experimental methods for the large molecules such as commercial dyes. In this context, to calculate theoretical dipole moments the current trend using computational chemistry methods has been increasing in many experimental interests such as molecular design, molecular modeling, dynamic simulation, structure analyzing and so on. In this experiment, the electric

dipole moments of the selected dyes were obtained using molecular modeling software, *CS Chem3D^{TM} Pro* (CambridgeSoft Co. USA) which is most frequently used for theoretical purposes. Although the computed results are not entirely exact, a quantitative or approximate computation results can give useful insight into chemistry.

References

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